TECHNOLOGY NEEDS/OPPORTUNITIES STATEMENT

DEVELOP DESCRIPTIONS OF CONTAMINANT FLOW AND TRANSPORT IN THE VADOSE ZONE

Identification No.: RL-SS29
Date: September 2001

Program: Environmental Restoration
OPS Office/Site: Richland Operations Office/Hanford Site
Operable Unit(s): Broad need potentially applicable to multiple operable units.
PBS No.: RL-SS04 (RL-VZ01)
Waste Stream: Disposition Map Designations: ER-04 [technical risk score 3], ER-14 [technical risk score 5], ER-03 [technical risk score 3]
TSD Title: N/A
Waste Management Unit (if applicable): N/A
Facility: N/A

***Priority Rating*:**

This entry addresses the "Accelerated Cleanup: Paths to Closure (ACPC)" priority:

X 1. Critical to the success of the ACPC
____ 2. Provides substantial benefit to ACPC projects (e.g., moderate to high lifecycle cost savings or risk reduction, increased likelihood of compliance, increased assurance to avoid schedule delays)
____ 3. Provides opportunities for significant, but lower cost savings or risk reduction, and may reduce uncertainty in ACPC project success.

***Need Title*:** Develop Descriptions of Contaminant Flow and Transport in the Vadose Zone.

Need/Opportunity Category: Technology Need

***Need Description*:** This need addresses specific technical gaps identified in the scope of the Groundwater/Vadose Zone Integration Project (Integration Project) at the Hanford Site and is written as an "integrated" need. The Integration Project is focused on providing the scientific and technical basis to ensure that Hanford Site decisions, including decisions related to long-term stewardship, are defensible and possess an integrated perspective for the protection of water resources, the Columbia River, river-dependent life, and users of the Columbia River resources. As such, this "integrated" need has both applied S&T components that are interrelated in addressing the specified technical gap. Individual efforts applied to resolve the technical gaps described in this need may address all or part of the components identified for this need. Where a specific technology need can be defined separately from an "integrated" need, a specific technology need statement has been written and is included elsewhere in the Hanford Site STCG Subsurface Contamination Needs (e.g., RL-SS25: Improved, Cost-Effective Methods for Subsurface Access to Support Characterization and Remediation).

The approach to date has been to use relatively simple models to describe contaminant transport in the vadose zone. These models are "simple" in that they lump many of the complexities into relatively few input parameters. For example, the potentially complex aspects of fluid chemistry and mineralogy are treated with a sorption coefficient and a porosity. The complexities of flow are described with two dispersion coefficients. Soil hydrological properties are allowed to change only with depth. Recharge rates, and consequently flow, are assumed to be constant with time rather than episodic, and coarse gridding for numerical models tends to smooth the calculated flow and mask the potential creation of fast paths in the real world. The sum of all of these simplifications and approximations is that the resultant calculated contaminant mobility is subject to very large errors. Furthermore, predictions made with these models cannot hold up to critical technical scrutiny, and more importantly, they fail to match observations that have and will be made by monitoring and characterization activities.

Previously employed approaches for modeling vadose zone transport do not capture essential processes that affect contaminant migration at Hanford. Previous modeling efforts have used decoupled approaches even though radionuclide and contaminant transport may involve fully coupled thermal-hydrological-mechanical-chemical processes. In addition, the effect of chemical coupling (through fluid density modification and mineral/precipitation dissolution) on fluid flow and radionuclide transport have been ignored. These types of simplifications may introduce unacceptable errors to long-term assessment of contaminant transport. Preferential flow in particular is considered to be an important contaminant transport mechanism in the Hanford vadose zone.

Improvement in modeling of vadose zone transport requires developing models which can capture the important complexities. This development will take the form of enhancing existing codes to represent additional processes, running them with finer grids and time spacings, and simulating some of the heterogeneities and episodicities. Partial coupling of physical and chemical processes may also be needed. It is expected that some potentially complicating processes can be demonstrated to be insignificant, and that the transport behavior produced in the complex models can be abstracted into more highly parameterized models for sitewide assessment and long term predictions.

The specific technical gaps associated with modeling of contaminant transport in the vadose zone are:

- Information is needed to assess the effects of high ionic strength aqueous solutions under varying redox and pH conditions present in some of the leaking storage tanks on the rate of metal/radionuclide migration. Although it is known that high ionic strength solutions change the partitioning behavior of strongly sorbed nuclides, especially alkalis like ^{137}Cs, it is not known quantitatively for a range of likely conditions, nor is it known how fast fluids are neutralized by reaction with the soil matrix, how much this fluid-rock interaction changes the sorption properties of the matrix, and whether the high densities of fluids cause them to flow downward fast enough that the effective surface area for sorption is

greatly reduced. A further concern is with non-isothermal effects near the tanks, and in the seepage of highly radioactive tank fluids.

- Techniques are needed to estimate flow, transport, and reaction/interaction parameters from data collected at different scales of observation and for transferring geo-hydrological information from one site to another with an understanding of the limitations of these techniques. These are long standing issues in hydrological modeling, but the approach used needs to be tailored to the type of system being modeled, and there needs to be enough data to estimate what sacrifices in terms of uncertainty are being made by using data measured at one scale to represent larger and smaller scales.

- Techniques are needed to adequately account for spatial and temporal heterogeneity that impacts contaminant transport. There is a need to model water seepage, and associated mass transport, on the actual scale on which these processes are taking place. This may require spatial resolution of order 0.1 - 1 m, and temporal resolution of order 1 hr - 1 day. How such resolution can be reconciled with site-wide modeling and assessment on time scales of 10 - 100 yr is a major challenge. The episodic nature of seepage, and associated hysteresis and mixing effects must also be accounted for. Episodic and intermittent features can come into play from the nature of precipitation and runoff, from tank leaks, and when considering sluicing to remove tank contents. The temporal structure of unsaturated zone seepage may be as important as the spatial structure (Science Needs RL-WT044-S).

- Improved multiphase-multicomponent reactive transport models that adequately describe contaminant migration in the Hanford vadose zone are needed. These models should include groups of specialized submodels relating to specific waste chemistry and other features that support site-specific and provide a basis for site-wide assessments. Current vadose zone modeling uses decoupled approaches. There are some process aspects (chemical reaction-induced changes in porosity, permeability, reactive surface area) that can only be captured through fully coupled modeling.

- Approaches for considering and incorporating uncertainty in transport modeling is needed to better communicate what is or is not known. This is also a widely appreciated aspect of hydrological modeling, but there are many possible approaches, and one or more need to be developed, decided upon and gain the acceptance of the concerned community.

- Information is needed to understand which secondary minerals form as colloids in groundwater, the importance of biosorption, the nature of the chemical interactions between contaminants of interest and the surfaces of inorganic and organic colloids, and the effect of colloids on contaminant transport at Hanford (Science Need RL-SS28-S).

- Information is needed to understand how the physical and chemical properties of the specific Hanford formations affect the transport of chemical solutes and colloids (Science Need RL-SS29-S).

- Techniques and information are needed to quantify the migration rate of contaminants through the vadose zone. Model formulations are needed for the chemistry and physics that describe the dispersal and longevity of subsurface contaminant plumes for site conditions, contaminant chemistry and reactivity, and hydraulic properties at Hanford (Science Need RL-SS31-S). The evolution of the present distribution of contaminants, both radioactive and nonradioactive (particularly ^{137}Cs but also Pu, ^{99}Tc, ^{90}Sr, Cr, CCl_4, and nitrate), beneath the tank farms and past practice disposal sites and to evaluate their potential mobility under all "leave or retrieve" options needs to be understood and quantified (Science Need RL-WT053-S). Techniques are needed to use readily measured chemical analogues (similar group, charge, ionic size) to contaminants of interest to assess the behavior of difficult-to-measure contaminants in the Hanford subsurface (Science Need RL-SS35-S).

Schedule Requirements:

Earliest Date Required: 8/1/99

Latest Date Required: 9/30/05

The Integration Project S&T Roadmap (DOE/RL-98-48, 2000) indicates the information that is required over the next 6 years to meet the objectives of the Integration Project. Information associated with descriptions contaminant transport in the vadose zone is needed in the FY99 to FY03 timeframe to meet these objectives.

***Problem Description*:** This need falls under the Vadose Zone Technical Element within the S&T Endeavor. The Vadose Zone Technical Element is intended to address and resolve scientific problems related to the leakage of radioactive and hazardous wastes into Hanford soils and sediments. The objective of the Vadose Zone Technical Element is to enhance protection of human health and the environment by providing 1) improved models, measurements, and data to predict contaminant migration and provide warning of potential surface or groundwater contamination before problems arise; 2) scientific rigor to system assessment and PA models as they are developed, reviewed, and implemented; and 3) scientific support for selection of the most safe, efficient, and effective remedial actions and site closure activities. An implicit goal of this research is to provide scientific and regulatory credibility to DOE's environmental management decision-making process.

The scope of this technical element encompasses the unsaturated zone beneath the Hanford Site. The geographic focus is on areas that (1) underlie liquid waste disposal sites; (2) have the potential for leaks or leaching; and (3) have experienced past leaks and spills. Also included are

selected areas away from the focus areas, such as areas representative of background conditions, and areas that have the potential to become contaminated in the future.

Specific topics for this need include (1) scientifically defensible predictive tools and (2) detailed process-level reactive transport models to provide a foundation for site-scale models for site-wide assessments.

Benefit to the Project Baseline of Filling Need: The application of surface barriers and other remediation strategies currently planned for the Hanford Site depends on improved measurements of transport processes in the vadose zone. Confidence in predicting contaminant travel times at treated or covered sites will be enhanced by implementing this activity. Successful completion of these activities is required to meet the objectives of the Integration Project and the related elements of the Paths to Closure.

***Functional Performance Requirements*:** The techniques applied or information that is obtained must describe and quantify contaminant transport in the Hanford vadose zone or provide relevant parameters or mathematical formulations such that the information can be applied toward the conceptual models, fate and transport numerical models, and system assessment capabilities that are being developed as part of the Integration Project.

Work Breakdown Structure (WBS) No.* :** 1.4.03.4.4 ***TIP No.: TIP-0012

Relevant PBS Milestone: PBS-MC-042

***Justification For Need*:**

Technical: Previously employed approaches for modeling vadose zone transport do not capture essential processes that affect contaminant migration at Hanford. Previous modeling efforts have used decoupled approaches even though radionuclide and contaminant transport may involve fully coupled thermal-hydrological-mechanical-chemical processes. In addition, the effect of chemical coupling (through fluid density modification and mineral/precipitation dissolution) on fluid flow and radionuclide transport have been ignored. These types of simplifications may introduce unacceptable errors to long-term assessment of contaminant transport.

Regulatory: Information obtained by addressing this need will provide an improved technical basis for making site regulatory decisions and therefore reduce the uncertainty associated with the basis for these decisions.

Environmental Safety & Health: This need addresses broad sitewide technical issues and, as such, crosscuts multiple applications that each may have specific environmental safety and health issues.

Potential Life-Cycle Cost Savings of Need (in $000s) and Cost Savings Explanation: The estimated life-cycle cost savings associated with filling this need is $200M. This estimate is based on an assumed savings of 5% of the total Hanford remediation life-cycle

cost of >$5B. Estimated savings are due to information and data gained by filling this need that supports decisions for cost effective remediation and long-term stewardship.

Cultural/Stakeholder Concerns: This technology need supports the resolution of cultural and stakeholder concerns as expressed by the CRCIA Team in "Columbia River Comprehensive Impact Assessment, Part II: Requirements for a Columbia River Comprehensive Impact Assessment" (DOE 1998).

Other: None

Current Baseline Technology: N/A

End-User: Richland Environmental Restoration Project

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DOE End-User/Representative Point-of-Contact: John G. Morse, DOE-RL, (509) 376-0057

Reference:

United States Department of Energy. 1998. Columbia River Comprehensive Impact Assessment, Part II; Requirements for a Columbia River Comprehensive Impact Assessment. DOE/RL-96-16. United States Department of Energy, Richland, Washington.

United States Department of Energy. 2000. Groundwater/Vadose Zone Integration Project Science and Technology Summary Description. DOE/RL-98-48, Vol. III, Rev. 1, U.S. Department of Energy, Richland, Washington.